Supplementary information

Zirconium Complexes of Cyclopenta[*b*]pyridine:

Synthesis, Structure, and Olefin Polymerization Catalysis †

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Jo Ann M. Canich,[b] Lyudmila G. Kuz'mina,[c] Judith A. K. Howard [d]

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Characterization data

1-(Trimethylsilyl)-1*H*-cyclopenta[*b*]pyridine (1). Anal. calc. for $C_{11}H_{15}NSi$: C, 69.78; H, 7.99. Found: C, 70.11; H, 8.08. ^{1}H NMR ($CDCl_3$): δ 8.03 (dt, J= 7.33 Hz, J= 1.17 Hz, 1H, 4-H in Cp^{Py}), 7.55 (dd, J= 6.15 Hz, J= 0.59 Hz, 1H, 2-H in Cp^{Py}), 7.37 (dd, J= 4.10 Hz, J = 3.51 Hz, 1H, 6-H in Cp^{Py}), 6.63 (dd, J= 7.32 Hz, J= 6.15 Hz, 1H, 3-H in Cp^{Py}), 6.53 (dd, J= 4.69 Hz, J= 1.46 Hz, 1H, 7-H in Cp^{Py}), 6.26 (dt, J= 3.51 Hz, J= 1.18 Hz, 1H, 5-H in Cp^{Py}), 0.71 (s, 9H, Me_3Si). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 147.6, 130.6, 130.3, 128.8, 119.1, 105.5, 99.1, 92.5, 0.8.

$Cp^{Py}Li$. ^{1}H NMR (THF-d_8): δ 7.52 (ddd, J= 7.52 Hz, J= 1.36 Hz, J= 1.03 Hz, 1H, 2-H in Cp^{Py}), 7.48 (dd, J= 4.78 Hz, J= 1.36 Hz, 1H, 4-H in Cp^{Py}), 6.81 (t, J= 3.76 Hz, 1H, 6-H in Cp^{Py}), 6.22 (dd, J= 7.52 Hz, J= 4.79 Hz, 1H, 3-H in Cp^{Py}), 5.86-5.89 (m, 2H, 5,7-H_2 in Cp^{Py}).

Cp*$ZrCl_3$. Anal. calc. for $C_{10}H_{15}Cl_3Zr$: C, 36.09; H, 4.54. Found: C, 36.13; H, 4.50. ^{1}H NMR ($C_6D_5CD_3$): δ 2.17 (s, $\Delta\nu_{1/2}$= 12.0 Hz, C_5*Me*$_5$). $^{13}C\{^1H\}$NMR ($C_6D_5CD_3$): δ 130.45 (*C*$_5Me_5$), 13.31 (C_5*Me*$_5$).

Cp^{Py}Cp*$ZrCl_2$ (2). Anal. calc. for $C_{18}H_{21}NCl_2Zr$: C, 52.28; H, 5.12. Found: C, 52.44; H, 5.04. ^{1}H NMR (CD_2Cl_2): 8.69 (dd, J= 4.15 Hz, J= 1.46 Hz, 1H, 2-H in Cp^{Py}), 7.93 (ddd, J= 8.55 Hz, J= 1.47 Hz, J= 0.98 Hz, 1H, 4-H in Cp^{Py}), 7.08 (dd, J= 8.54 Hz, J= 4.15 Hz, 1H, 3-H in Cp^{Py}), 6.41 (dd, J= 3.91 Hz, J= 3.17 Hz, 1H, 6-H in Cp^{Py}), 6.32 (dd, J= 3.90 Hz, J= 2.20 Hz, 1H, 7-H in Cp^{Py}), 6.23 (ddd, J= 3.17 Hz, J= 2.19 Hz, J= 0.98 Hz, 1H, 5-H in Cp^{Py}), 2.00 (s, 15H, Cp*). $^{13}C\{^1H\}$ NMR (CD_2Cl_2):[10] δ 152.3 (2-C in Cp^{Py}), 145.8 (8-C in Cp^{Py}), 133.1 (4-C in Cp^{Py}),

127.3 (9-C in Cp^{Py}), 124.5 (C_5Me_5), 119.9 (3-C in Cp^{Py}), 115.9 (6-C in Cp^{Py}), 105.7 (7-C in Cp^{Py}), 99.8 (5-C in Cp^{Py}), 12.0 (C_5Me_5).

$Cp^{Py}Zr(NMe_2)_3(NHMe_2)$ (3). Anal. calc. for $C_{16}H_{31}N_5Zr$: C, 49.96; H, 8.12. Found: C, 50.24; H, 8.19. ^1H NMR (CD_2Cl_2): at 20°C, δ 7.77 (d, J= 7.82 Hz, 1H, 2-H in Cp^{Py}), 7.61 (br.s, 1H, 4-H in Cp^{Py}), 6.92 (t, J= 3.67 Hz, 1H, 6-H in Cp^{Py}), 6.45 (dd, J= 7.57 Hz, J= 5.12 Hz, 1H, 3-H in Cp^{Py}), 6.11 (dd, J= 3.91 Hz, J= 1.46 Hz, 1H, 7-H in Cp^{Py}), 5.98 (br.s, 1H, 5-H in Cp^{Py}), 2.96 (br.s, 18H, $Zr(NMe_2)_3$), 2.33 (br.d, J= 6.45 Hz, 6H, $Zr(HNMe_2)$), Me_2NH resonance was not observed; at -75°C, δ 7.72 (d, J= 7.82 Hz, 1H, 2-H in Cp^{Py}), 7.46 (d, J= 4.63 Hz, 1H, 4-H in Cp^{Py}), 6.85 (br.t, J= 3.67 Hz, 1H, 6-H in Cp^{Py}), 6.38 (dd, J= 7.57 Hz, J= 5.12 Hz, 1H, 3-H in Cp^{Py}), 6.00 (d, J= 2.44 Hz, 1H, 7-H in Cp^{Py}), 5.79 (br.s, 1H, 5-H in Cp^{Py}), 2.92 (br.s, 18H, $Zr(NMe_2)_3$), 2.53 (br.s, 1H, $Zr(HNMe_2)$), 2.25 (br.s, 6H, $Zr(HNMe_2)$). $^{13}C\{^1H\}$ NMR (CD_2Cl_2, -75°C):[10] δ 142.6 (8-C in Cp^{Py}), 137.7 (2-C in Cp^{Py}), 128.4 (4-C in Cp^{Py}), 126.9 (9-C in Cp^{Py}), 125.1 (6-C in Cp^{Py}), 106.4 (3-C in Cp^{Py}), 95.9 (7-C in Cp^{Py}), 93.1 (5-C in Cp^{Py}), 43.1 ($Zr(NMe_2)_3$), 40.5 ($Zr(HNMe_2)$).

Computational data for 3

HyperChem log start -- Mon Nov 06 20:22:24 2000.

Geometry optimization, SemiEmpirical, molecule = C:\Program Files\Hyper5\Program\pyrZr_6.hin.

ZINDO1

PolakRibiere optimizer

Convergence limit = 0.0100000 Iteration limit = 50

Overlap weighting factors: P(Sigma-Sigma) = 1.0000 and P(Pi-Pi) = 1.0000

Accelerate convergence = YES

Optimization algorithm = Polak-Ribiere

Criterion of RMS gradient = 0.0100 kcal/(A mol) Maximum cycles = 795

UHF Calculation:

Singlet state calculation

Number of electrons = 124

in which

Number of Alpha Electrons = 62

Number of Beta Electrons = 62

Charge on the System = 0

Total Orbitals = 124

Starting ZINDO/1 calculation with 124 orbitals

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=1 Diff=37363.78299]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=2 Diff=366.24971]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=3 Diff=32.89089]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=4 Diff=72.41715]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=5 Diff=77.73457]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=6 Diff=26.98125]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=7 Diff=3.34018]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=8 Diff=0.27395]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=9 Diff=0.02895]

E=0.0000 Grad=0.000 Conv=NO(0 cycles 0 points) [Iter=10 Diff=0.00402]

E=-14189.0908 Grad=0.015 Conv=NO(0 cycles 1 points) [Iter=1 Diff=0.00005]

E=-14189.0908 Grad=0.013 Conv=NO(0 cycles 2 points) [Iter=1 Diff=0.00000]

E=-14189.0908 Grad=0.014 Conv=NO(0 cycles 3 points) [Iter=1 Diff=0.00000]

E=-14189.0908 Grad=0.007 Conv=YES(1 cycles 4 points) [Iter=1 Diff=0.00000]

ENERGIES AND GRADIENT

Total Energy = -113835.7533673 (kcal/mol)

Total Energy = -181.405198203 (a.u.)

Binding Energy = -14189.0907314 (kcal/mol)

Isolated Atomic Energy = -99646.6626359 (kcal/mol)

Electronic Energy = -803348.1579997 (kcal/mol)

Core-Core Interaction = 689512.4046324 (kcal/mol)

Heat of Formation = -9129.1887314 (kcal/mol)

Gradient = 0.0075245 (kcal/mol/Ang)

MOLECULAR POINT GROUP

C1 >

EIGENVALUES(eV)

Alpha Orbitals:

Symmetry:	1 A	2 A	3 A	4 A	5 A
Eigenvalue:	-54.567356	-48.324810	-46.871426	-43.839657	-42.750843
Symmetry:	6 A	7 A	8 A	9 A	10 A
Eigenvalue:	-41.596039	-38.537838	-34.555733	-33.443981	-32.512543
Symmetry:	11 A	12 A	13 A	14 A	15 A
Eigenvalue:	-31.670666	-31.035582	-29.990421	-28.973177	-27.281281
Symmetry:	16 A	17 A	18 A	19 A	20 A
Eigenvalue:	-25.931948	-25.488653	-24.162676	-24.050070	-23.826939
Symmetry:	21 A	22 A	23 A	24 A	25 A
Eigenvalue:	-23.712851	-22.954769	-22.669741	-21.661386	-20.331520
Symmetry:	26 A	27 A	28 A	29 A	30 A
Eigenvalue:	-19.805887	-19.633438	-19.474733	-18.877392	-18.069117
Symmetry:	31 A	32 A	33 A	34 A	35 A
Eigenvalue:	-18.033173	-17.965025	-17.366579	-17.085218	-16.568018
Symmetry:	36 A	37 A	38 A	39 A	40 A
Eigenvalue:	-16.527809	-16.238716	-15.447005	-14.852564	-14.365267
Symmetry:	41 A	42 A	43 A	44 A	45 A
Eigenvalue:	-14.165562	-13.943611	-13.803857	-13.283681	-12.944793
Symmetry:	46 A	47 A	48 A	49 A	50 A
Eigenvalue:	-12.340197	-12.244691	-11.477256	-11.035009	-10.934182
Symmetry:	51 A	52 A	53 A	54 A	55 A
Eigenvalue:	-10.606629	-10.581017	-9.576185	-9.250910	-8.677772
Symmetry:	56 A	57 A	58 A	59 A	60 A
Eigenvalue:	-8.100236	-7.932530	-7.413867	-6.993096	-6.268547
Symmetry:	61 A	62 A	63 A	64 A	65 A
Eigenvalue:	-5.732939	-5.271911	4.399101	5.249022	5.516120
Symmetry:	66 A	67 A	68 A	69 A	70 A
Eigenvalue:	5.718116	5.997530	6.789362	7.269477	7.766924
Symmetry:	71 A	72 A	73 A	74 A	75 A
Eigenvalue:	7.982682	8.051976	8.630852	9.811058	10.077785
Symmetry:	76 A	77 A	78 A	79 A	80 A
Eigenvalue:	10.198258	10.638333	10.915113	11.271956	11.292853
Symmetry:	81 A	82 A	83 A	84 A	85 A
Eigenvalue:	11.569613	11.742179	11.976271	12.305321	12.410294

Symmetry: 86 A 87 A 88 A 89 A 90 A

Eigenvalue: 12.476222 12.626031 12.729144 12.902426 12.943390

Symmetry: 91 A 92 A 93 A 94 A 95 A

Eigenvalue: 13.078467 13.267961 13.413451 13.487084 13.579250

Symmetry: 96 A 97 A 98 A 99 A 100 A

Eigenvalue: 13.683575 13.879293 14.108225 14.163854 14.327675

Symmetry: 101 A 102 A 103 A 104 A 105 A

Eigenvalue: 14.339141 14.362899 14.417199 14.505264 14.659489

Symmetry: 106 A 107 A 108 A 109 A 110 A

Eigenvalue: 14.730571 14.840830 14.915606 15.025861 15.052179

Symmetry: 111 A 112 A 113 A 114 A 115 A

Eigenvalue: 15.069099 15.160592 15.266713 15.560788 15.658899

Symmetry: 116 A 117 A 118 A 119 A 120 A

Eigenvalue: 15.877993 16.150078 16.652456 17.210381 17.231588

Symmetry: 121 A 122 A 123 A 124 A

Eigenvalue: 17.293137 17.306273 17.758524 18.690790

Beta Orbitals:

Symmetry: 1 A 2 A 3 A 4 A 5 A

Eigenvalue: -54.567356 -48.324810 -46.871426 -43.839657 -42.750843

Symmetry: 6 A 7 A 8 A 9 A 10 A

Eigenvalue: -41.596039 -38.537838 -34.555733 -33.443981 -32.512543

Symmetry: 11 A 12 A 13 A 14 A 15 A

Eigenvalue: -31.670666 -31.035582 -29.990421 -28.973177 -27.281281

Symmetry: 16 A 17 A 18 A 19 A 20 A

Eigenvalue: -25.931948 -25.488653 -24.162676 -24.050070 -23.826939

Symmetry: 21 A 22 A 23 A 24 A 25 A

Eigenvalue: -23.712851 -22.954769 -22.669741 -21.661386 -20.331520

Symmetry: 26 A 27 A 28 A 29 A 30 A

Eigenvalue: -19.805887 -19.633438 -19.474733 -18.877392 -18.069117

Symmetry: 31 A 32 A 33 A 34 A 35 A

Eigenvalue: -18.033173 -17.965025 -17.366579 -17.085218 -16.568018

Symmetry: 36 A 37 A 38 A 39 A 40 A

Eigenvalue: -16.527809 -16.238716 -15.447005 -14.852564 -14.365267

Symmetry: 41 A 42 A 43 A 44 A 45 A

Eigenvalue:	-14.165562	-13.943611	-13.803857	-13.283681	-12.944793
Symmetry:	46 A	47 A	48 A	49 A	50 A
Eigenvalue:	-12.340198	-12.244691	-11.477255	-11.035009	-10.934182
Symmetry:	51 A	52 A	53 A	54 A	55 A
Eigenvalue:	-10.606629	-10.581017	-9.576185	-9.250910	-8.677771
Symmetry:	56 A	57 A	58 A	59 A	60 A
Eigenvalue:	-8.100235	-7.932529	-7.413866	-6.993096	-6.268546
Symmetry:	61 A	62 A	63 A	64 A	65 A
Eigenvalue:	-5.732939	-5.271910	4.399101	5.249022	5.516120
Symmetry:	66 A	67 A	68 A	69 A	70 A
Eigenvalue:	5.718115	5.997530	6.789362	7.269477	7.766924
Symmetry:	71 A	72 A	73 A	74 A	75 A
Eigenvalue:	7.982682	8.051976	8.630852	9.811058	10.077785
Symmetry:	76 A	77 A	78 A	79 A	80 A
Eigenvalue:	10.198258	10.638333	10.915113	11.271956	11.292853
Symmetry:	81 A	82 A	83 A	84 A	85 A
Eigenvalue:	11.569613	11.742180	11.976271	12.305321	12.410294
Symmetry:	86 A	87 A	88 A	89 A	90 A
Eigenvalue:	12.476222	12.626031	12.729144	12.902426	12.943390
Symmetry:	91 A	92 A	93 A	94 A	95 A
Eigenvalue:	13.078467	13.267961	13.413451	13.487083	13.579250
Symmetry:	96 A	97 A	98 A	99 A	100 A
Eigenvalue:	13.683575	13.879293	14.108225	14.163853	14.327677
Symmetry:	101 A	102 A	103 A	104 A	105 A
Eigenvalue:	14.339141	14.362899	14.417199	14.505264	14.659489
Symmetry:	106 A	107 A	108 A	109 A	110 A
Eigenvalue:	14.730571	14.840830	14.915606	15.025861	15.052179
Symmetry:	111 A	112 A	113 A	114 A	115 A
Eigenvalue:	15.069099	15.160592	15.266713	15.560788	15.658899
Symmetry:	116 A	117 A	118 A	119 A	120 A
Eigenvalue:	15.877993	16.150078	16.652456	17.210381	17.231588
Symmetry:	121 A	122 A	123 A	124 A	
Eigenvalue:	17.293137	17.306273	17.758524	18.690790	

ATOMIC ORBITAL ELECTRON POPULATIONS

Alpha Orbitals:

AO:	16 S Zr	16 Px Zr	16 Py Zr	16 Pz Zr	16 Dz2 Zr
	0.218373	0.192878	0.206867	0.141032	0.180695
AO:	16 Dxz Zr	16 Dyz Zr	16 Dx2 Zr	16 Dxy Zr	2 S C
	0.235940	0.222744	0.226018	0.230465	0.527612
AO:	2 Px C	2 Py C	2 Pz C	3 S C	3 Px C
	0.507487	0.491680	0.538447	0.533566	0.475349
AO:	3 Py C	3 Pz C	4 S N	4 Px N	4 Py N
	0.475767	0.442355	0.755521	0.718591	0.536228
AO:	4 Pz N	5 S C	5 Px C	5 Py C	5 Pz C
	0.623876	0.512638	0.478657	0.449701	0.475184
AO:	6 S C	6 Px C	6 Py C	6 Pz C	7 S C
	0.508076	0.508359	0.474197	0.516195	0.521513
AO:	7 Px C	7 Py C	7 Pz C	8 S C	8 Px C
	0.504296	0.492896	0.517181	0.522242	0.498647
AO:	8 Py C	8 Pz C	9 S C	9 Px C	9 Py C
	0.484841	0.492993	0.524151	0.481648	0.497807
AO:	9 Pz C	1 S C	1 Px C	1 Py C	1 Pz C
	0.546730	0.529834	0.474758	0.511102	0.472623
AO:	17 S N	17 Px N	17 Py N	17 Pz N	18 S N
	0.635800	0.555023	0.833029	0.596067	0.633832
AO:	18 Px N	18 Py N	18 Pz N	19 S N	19 Px N
	0.800722	0.565668	0.631495	0.638631	0.672156
AO:	19 Py N	19 Pz N	20 S N	20 Px N	20 Py N
	0.581431	0.746325	0.641372	0.769986	0.586446
AO:	20 Pz N	21 S C	21 Px C	21 Py C	21 Pz C
	0.565967	0.525758	0.496574	0.504310	0.473022
AO:	22 S C	22 Px C	22 Py C	22 Pz C	24 S C
	0.528340	0.466759	0.505326	0.502925	0.541032
AO:	24 Px C	24 Py C	24 Pz C	25 S C	25 Px C
	0.517468	0.463573	0.516824	0.532216	0.497781
AO:	25 Py C	25 Pz C	26 S C	26 Px C	26 Py C
	0.492718	0.501522	0.527415	0.483299	0.495608

AO: 26 Pz C 27 S C 27 Px C 27 Py C 27 Pz C
0.491809 0.526613 0.498388 0.473466 0.500304
AO: 28 S C 28 Px C 28 Py C 28 Pz C 29 S C
0.521447 0.497804 0.490268 0.485591 0.534361
AO: 29 Px C 29 Py C 29 Pz C 23 S H 11 S H
0.503082 0.472537 0.503478 0.424357 0.475025
AO: 12 S H 13 S H 14 S H 15 S H 10 S H
0.482407 0.472984 0.463117 0.472346 0.489291
AO: 30 S H 31 S H 32 S H 33 S H 34 S H
0.496298 0.489124 0.494947 0.494700 0.495700
AO: 35 S H 36 S H 37 S H 38 S H 39 S H
0.494009 0.492087 0.468246 0.498140 0.499654
AO: 40 S H 41 S H 42 S H 43 S H 44 S H
0.473870 0.491437 0.495675 0.500560 0.495194
AO: 45 S H 46 S H 47 S H 48 S H 49 S H
0.499625 0.496215 0.500041 0.484749 0.477055
AO: 50 S H 51 S H 52 S H 53 S H
0.468111 0.483685 0.470356 0.457664

Beta Orbitals:

AO: 16 S Zr 16 Px Zr 16 Py Zr 16 Pz Zr 16 Dz2 Zr
0.218373 0.192878 0.206867 0.141032 0.180696
AO: 16 Dxz Zr 16 Dyz Zr 16 Dx2 Zr 16 Dxy Zr 2 S C
0.235940 0.222744 0.226018 0.230465 0.527612
AO: 2 Px C 2 Py C 2 Pz C 3 S C 3 Px C
0.507487 0.491680 0.538447 0.533566 0.475349
AO: 3 Py C 3 Pz C 4 S N 4 Px N 4 Py N
0.475767 0.442356 0.755521 0.718591 0.536228
AO: 4 Pz N 5 S C 5 Px C 5 Py C 5 Pz C
0.623875 0.512638 0.478657 0.449701 0.475185
AO: 6 S C 6 Px C 6 Py C 6 Pz C 7 S C
0.508076 0.508359 0.474197 0.516195 0.521513
AO: 7 Px C 7 Py C 7 Pz C 8 S C 8 Px C
0.504296 0.492896 0.517181 0.522242 0.498647
AO: 8 Py C 8 Pz C 9 S C 9 Px C 9 Py C

0.484841 0.492993 0.524151 0.481648 0.497807

AO: 9 Pz C 1 S C 1 Px C 1 Py C 1 Pz C

0.546730 0.529834 0.474758 0.511102 0.472624

AO: 17 S N 17 Px N 17 Py N 17 Pz N 18 S N

0.635800 0.555023 0.833029 0.596067 0.633832

AO: 18 Px N 18 Py N 18 Pz N 19 S N 19 Px N

0.800722 0.565668 0.631495 0.638631 0.672156

AO: 19 Py N 19 Pz N 20 S N 20 Px N 20 Py N

0.581431 0.746325 0.641372 0.769986 0.586446

AO: 20 Pz N 21 S C 21 Px C 21 Py C 21 Pz C

0.565967 0.525758 0.496574 0.504310 0.473022

AO: 22 S C 22 Px C 22 Py C 22 Pz C 24 S C

0.528340 0.466759 0.505326 0.502925 0.541032

AO: 24 Px C 24 Py C 24 Pz C 25 S C 25 Px C

0.517468 0.463573 0.516824 0.532216 0.497781

AO: 25 Py C 25 Pz C 26 S C 26 Px C 26 Py C

0.492718 0.501522 0.527415 0.483299 0.495608

AO: 26 Pz C 27 S C 27 Px C 27 Py C 27 Pz C

0.491809 0.526613 0.498388 0.473466 0.500304

AO: 28 S C 28 Px C 28 Py C 28 Pz C 29 S C

0.521447 0.497804 0.490268 0.485591 0.534362

AO: 29 Px C 29 Py C 29 Pz C 23 S H 11 S H

0.503082 0.472537 0.503479 0.424356 0.475025

AO: 12 S H 13 S H 14 S H 15 S H 10 S H

0.482407 0.472984 0.463117 0.472346 0.489291

AO: 30 S H 31 S H 32 S H 33 S H 34 S H

0.496298 0.489124 0.494947 0.494700 0.495700

AO: 35 S H 36 S H 37 S H 38 S H 39 S H

0.494009 0.492087 0.468246 0.498140 0.499654

AO: 40 S H 41 S H 42 S H 43 S H 44 S H

0.473870 0.491437 0.495675 0.500560 0.495194

AO: 45 S H 46 S H 47 S H 48 S H 49 S H

0.499625 0.496215 0.500041 0.484749 0.477055

AO: 50 S H 51 S H 52 S H 53 S H

0.468111 0.483685 0.470356 0.457664

NET CHARGES AND COORDINATES

Atom	Z	Charge	Coordinates(Angstrom) x	y	z	Mass
Zr(16)	40	0.289976	-0.57741	0.71278	-0.47903	91.22000
C(2)	6	-0.130453	-0.63709	-2.57975	2.20895	12.01100
C(3)	6	0.145925	0.60393	-2.66750	1.51352	12.01100
N(4)	7	-0.268431	1.41196	-1.62895	1.26345	14.00700
C(5)	6	0.167640	0.83078	-0.38711	1.42968	12.01100
C(6)	6	-0.013654	-0.50502	-0.19124	1.97568	12.01100
C(7)	6	-0.071772	-0.73486	1.23852	2.04697	12.01100
C(8)	6	0.002554	0.44979	1.89413	1.60205	12.01100
C(9)	6	-0.100671	1.39763	0.91465	1.16385	12.01100
C(1)	6	0.023366	-1.22813	-1.35174	2.40875	12.01100
N(17)	7	-0.239839	1.02025	1.36720	-1.91791	14.00700
N(18)	7	-0.263433	-0.70415	-1.39491	-1.27119	14.00700
N(19)	7	-0.277086	-1.87722	2.50838	-0.99213	14.00700
N(20)	7	-0.127542	-3.13420	-0.06702	-0.08314	14.00700
C(21)	6	0.000672	0.55276	1.67675	-3.22858	12.01100
C(22)	6	-0.006699	2.42832	1.53369	-1.87024	12.01100
C(24)	6	-0.077793	-3.20324	-1.36865	0.50481	12.01100
C(25)	6	-0.048474	-3.87787	0.88230	0.68754	12.01100
C(26)	6	0.003736	-2.98451	2.48814	-1.88207	12.01100
C(27)	6	0.002457	-1.58629	3.84191	-0.59674	12.01100
C(28)	6	0.009780	-1.41861	-1.15304	-2.48125	12.01100
C(29)	6	-0.026919	-0.50538	-2.74665	-0.91348	12.01100
H(23)	1	0.151287	-3.53900	-0.09428	-1.05930	1.00800
H(11)	1	0.049951	-1.10657	-3.50196	2.56507	1.00800
H(12)	1	0.035186	-2.09327	-1.23829	3.07688	1.00800
H(13)	1	0.054032	-1.60023	1.72084	2.51271	1.00800
H(14)	1	0.073765	2.42631	1.11731	0.84794	1.00800
H(15)	1	0.055307	0.62723	2.97433	1.63862	1.00800
H(10)	1	0.021419	1.08684	-3.65240	1.41993	1.00800

H(30)	1	0.007405	0.99390	1.00724	-3.98768	1.00800
H(31)	1	0.021751	-0.54622	1.59160	-3.32696	1.00800
H(32)	1	0.010107	0.81781	2.70903	-3.51705	1.00800
H(33)	1	0.010600	2.94504	0.84181	-2.55753	1.00800
H(34)	1	0.008600	2.72852	2.55750	-2.15328	1.00800
H(35)	1	0.011981	2.82451	1.34576	-0.85677	1.00800
H(36)	1	0.015825	0.13084	-3.27441	-1.64416	1.00800
H(37)	1	0.063508	-0.00256	-2.82603	0.09122	1.00800
H(38)	1	0.003720	-1.45625	-3.30382	-0.83631	1.00800
H(39)	1	0.000693	-2.40287	-1.65562	-2.49828	1.00800
H(40)	1	0.052259	-1.62072	-0.06448	-2.65187	1.00800
H(41)	1	0.017126	-0.86157	-1.50391	-3.36749	1.00800
H(42)	1	0.008649	-1.34962	4.48722	-1.46050	1.00800
H(43)	1	-0.001119	-2.43948	4.30750	-0.07188	1.00800
H(44)	1	0.009612	-0.72230	3.88901	0.08965	1.00800
H(45)	1	0.000750	-3.87226	2.98462	-1.45021	1.00800
H(46)	1	0.007570	-2.75927	3.01042	-2.82908	1.00800
H(47)	1	-0.000083	-3.28965	1.45973	-2.15012	1.00800
H(48)	1	0.030503	-4.91986	0.56062	0.84282	1.00800
H(49)	1	0.045889	-3.41131	1.01895	1.67566	1.00800
H(50)	1	0.063778	-3.89134	1.85434	0.16516	1.00800
H(51)	1	0.032630	-4.22237	-1.62370	0.83533	1.00800
H(52)	1	0.059287	-2.86835	-2.13542	-0.21328	1.00800
H(53)	1	0.084672	-2.51403	-1.41774	1.38682	1.00800

Dipole (Debyes)	x	y	z	Total
Point-Chg.	-3.453	-1.630	3.197	4.980
sp Hybrid	-3.606	-0.010	-1.452	3.887
pd Hybrid	-0.297	-0.167	0.029	0.342
Sum	-7.356	-1.807	1.774	7.780